AR201-13461A

Table 1. Test Plan for C.I. Disperse Blue 79:1 (CAS No. 3618-72-2)

Endpoint	Data Available	Acceptable	Planned Testing
	Physical/Chemical Elements		
Melting Point	>/= 138° C	Yes	
Boiling Point	476° C (1)	Yes	
Vapor Pressure	$4.53X10^{-9}$ hPa @ 25° C (1)	Yes	
Partition coefficient	4.44@ 25°C	Yes	
Water solubility	5.2 µg/l @ 25°C	Yes	
	Environmental Fate and Pathways Elements		
Photodegredation	$T_{1/2}$ = 0.568 hr (EPIWIN)	Yes	
Stability in water	$T_{1/2}$ = </= 4 hr	Yes	
Fugacity	Sediment sorption	Yes	
Biodegredation	Anaerobic degredation	Yes	
	Ecotoxicity Elements		
Acute Toxicity/fish	NOEC > 4.8 µg/l	Yes	
Toxicity/aquatic plants	Algae (1)	Yes	
Acute toxicity/ aquatic invertebrates	Daphnia (1)	Yes	
	Health Elements		
Acute toxicity	MTD=2500 mg/kg/day	Yes	
Mutagenicity *in vitro*	Positive (Ames)	Yes	
Mutagenitcity *in vivo*	Negative (fruit fly)	Yes	
Repeat dose toxicity	NOAEL > 2500 mg/kg/day	Yes	
Reproductive toxicity	NOAEL > 2000 mg/kg/d (rat)	Yes	
	NOAEL > 100 mg/kg/d (rab)	Yes	
Teratogenicity	NOAEL > 2000 mg/kg/d (rat)	Yes	
	NOAEL > 300 mg/kg/day (rab)	Yes	

Notes

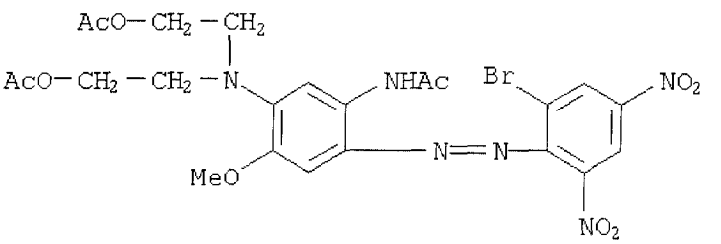
(1) Reported data are for related dye, C.I. Disperse Blue 79 (CAS No. 12239-34-8)

C.I. Disperse Blue 79:1
CAS No. 3618-72-2

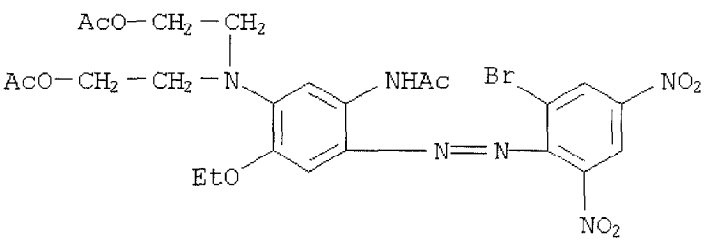
Test Plan Justification

C.I. Disperse Blue 79:1 (DB79:1) has been tested extensively as documented in the accompanying IUCLID robust summary and attached test plan. As a result of a voluntary test program conducted by U.S. dye makers, the EPA in 1993 declared that sufficient test data exist for DB79:1 to indicate relatively low toxicity and low concern for environmental risk, and that further work on DB79:1 was not justified (1). In fact, the agency removed DB79:1 from its Master Testing List in 1992 because it had received, reviewed, and accepted the results of all tests required under TSCA Section 4 (2).

In the few instances shown below where test data do not exist for DB79:1 (e.g., vapor pressure, toxicity/algae), data are provided for the close structural analog, C.I. Disperse Blue 79 (CAS No. 12239-34-8). The justification for using data on Disperse Blue 79 as surrogate data for DB79:1 is evident from examination of the similarity of their structures:



C.I. Disperse Blue 79:1. Chemical name: Acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-methoxyphenyl]-



C.I. Disperse Blue 79. Chemical name: Acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-ethoxyphenyl]-

The structures of these two related dyes are identical in every respect except for the 4-methoxyphenyl moiety in DB79:1 which is a 4-ethoxyphenyl moiety in Disperse Blue 79. One would anticipate that this slight change in chemical structure would have very little impact on the chemical, physical, and biological properties. In fact, the partition

coefficients of the two substances are virtually identical. For DB79:1, Log P_{ow} = 4.44, as documented in the attached test plan and robust summary, while for Disperse Blue 79 Log P_{ow} = 4.1 (3). Similarly, the water solubility of DB79:1 is 5.2 μg/l @ 25° C and for Disperse Blue 79 it is 5.4 μg/l @ 25° C (3).

Further similarities between the two structures are demonstrated by the EPIWIN modeling program recommended by the HPV Challenge Guidance. EPIWIN predicts an overall hydroxyl radical photodegradation rate constant for DB79:1 of 2.26 X 10^{-10} cm^3/molecule-sec, with a half-life of 0.568 hours at hydroxyl concentration of 1.5 X 10^6 molecules/cm^3. This compares to the predicted values for Disperse Blue 79 of a rate constant of 1.49 X 10^{-10} cm^3/molecule-sec, with a half-life of 0.863 hours at hydroxyl concentration of 1.5 X 10^6 molecules/cm^3 (4).

Physical/Chemical Elements. The physical/chemical properties of DB79:1 that are documented in the attached robust summary were obtained from the published scientific literature or manufacturer's material safety data sheet (MSDS). All reported data appear reliable and are based on standard methodology, so no additional testing is planned.

Environmental Fate and Pathways Elements. Valid experimental data on DB79:1 are reported in the attached robust summary for three of the four required HPV end points: stability in water, fugacity, and biodegradation. For photodegradation, the fourth required end point, data were modeled using the EPIWIN program, as recommended by the HPV Challenge Guidance.

DB79:1 is removed from effluent by the settling of particulate matter and adsorption on activated sludge. Complete removal of DB79:1 occurs through anaerobic degradation. No dye is found in sediment or water samples downstream from the wastewater treatment plant.

No data gaps exist requiring further testing.

Ecotoxicity Elements. Test results of a valid and very thorough acute fish toxicity test of DB79:1 are summarized in the attached robust summary and test plan. In this study, no toxicity of the dye was observed at concentrations up to the experimental limits of water solubility, > 4.8 μg/l. No data are available on DB79:1 specifically for toxicity in aquatic plants or aquatic invertebrates, but data are summarized for these two end points on the close structural relative, Disperse Blue 79. As explained above, these data are acceptable surrogates for DB79:1. Therefore, no additional testing is planned.

Health Elements. All HPV-required health endpoints for DB79:1 have been fulfilled satisfactorily by the results of previous studies conducted voluntarily by U.S. dye makers. These studies are documented in the attached robust summary and test plan.

DB79:1 is not toxic in rats by oral administration when administered in a 14-day acute study or in a 90-day repeated dose study at daily doses up to 2,500 mg/kg/bw. Although found to be positive in the Ames *Salmonella* bacterial mutagenicity assay, subsequent tests for genetic toxicity were negative in mammalian V79 cells, the mouse micronucleus assay, and the *Drosophila* (fruit fly) SLRL mutagenicity test.

Similarly, no reproductive toxicity or teratogenicity was observed in rats at doses up to 2,000 mg/kg/bw. In rabbits, some maternal toxicity and fetal body weight reduction were

observed at 300 and 600 mg/kg/bw, respectively, but there was no evidence of teratogenicity at any dose tested up to 600 mg/kg/bw.

Additional studies on the metabolism of DB79:1 in rats indicated that the dye is not extensively absorbed from the GI tract but is substantially cleared without undergoing any significant metabolism.

No further testing is necessary to satisfy the health-related endpoints for the HPV Challenge.

REFERENCES

1. EPA (January 11, 1993). Letter with attachments from C. Auer, U.S. Environmental Protection Agency, to Dr. C.T. Helmes, ETAD.
2. Master Testing List (December 1, 1992). Office of Pollution Prevention and Toxics, U.S. Environmental Protection Agency, Washington, DC.
3. Clariant (June 1996). IUCLID Dataset for C.I. Disperse Blue 79 (CAS No. 12239-34-8).
4. Meylan, W. and Howard, P. (2000). EPIWIN Modeling Program, Syracuse Research Corporation, Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510